Electronic Supplementary Information (ESI) for the article entitled:

Identification of anionic selenium species in Se-rich yeast by electrospray QTOF MS/MS and hybrid linear ion trap/Orbitrap MS^n

by Mihaly Dernovics, Johann Far and Ryszard Lobinski*

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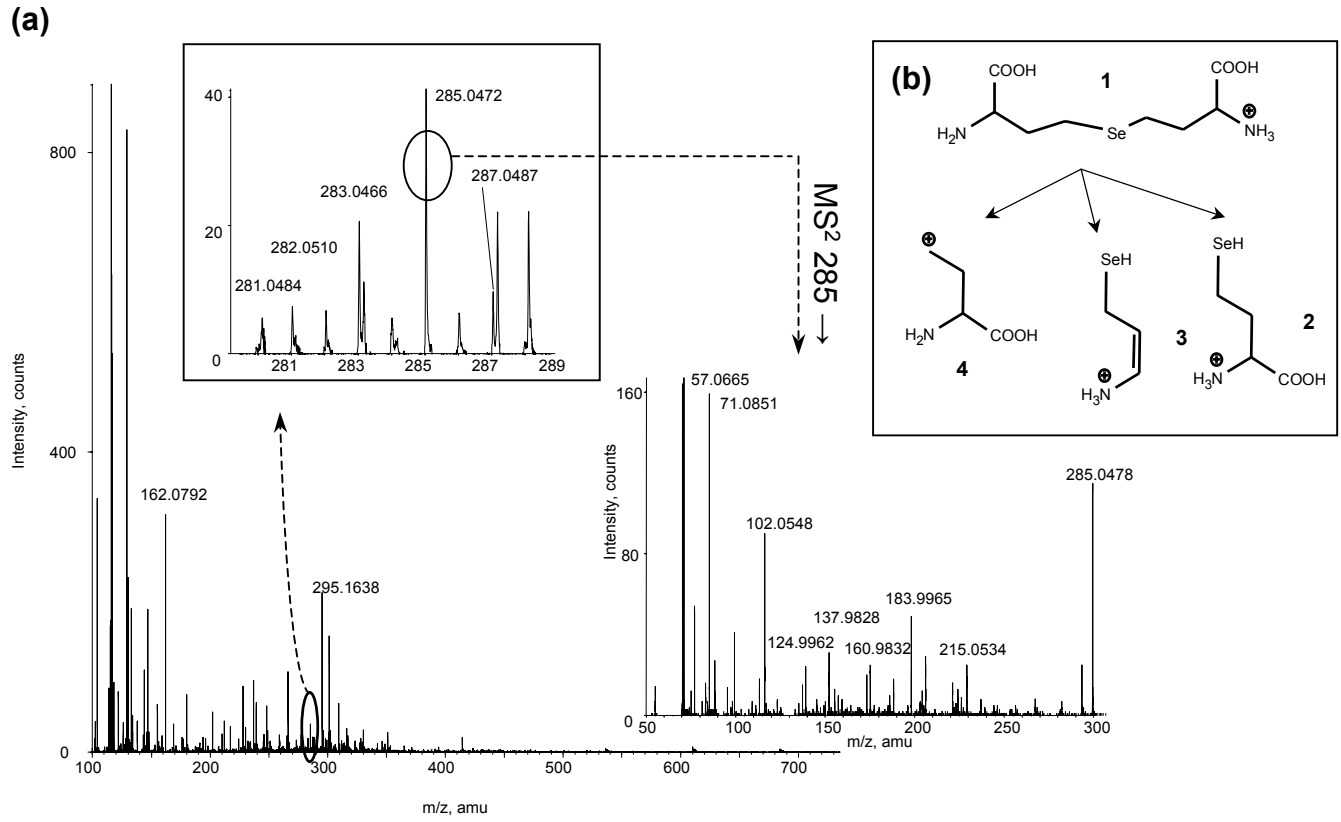
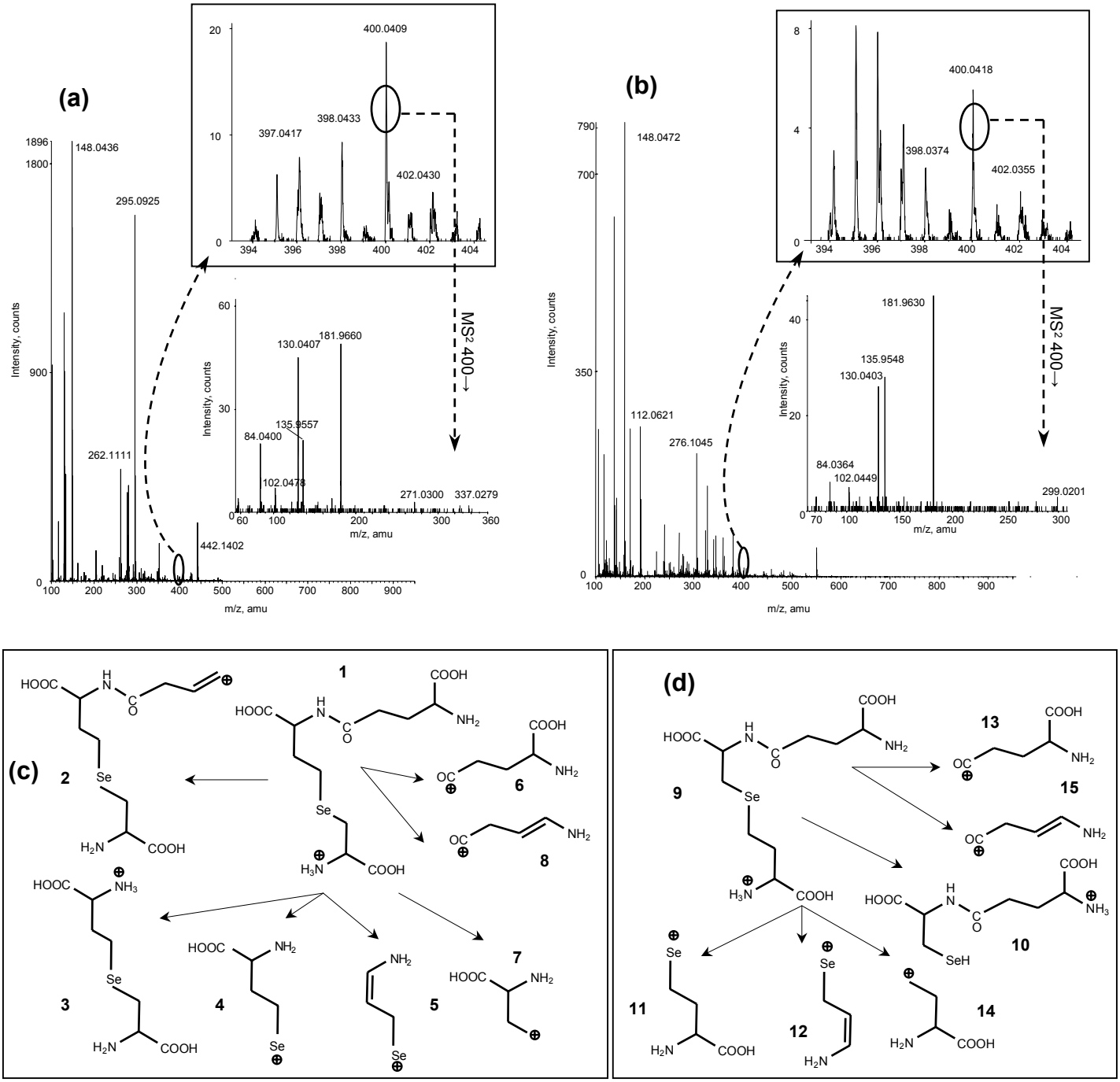
ESI Fig. 1



ESI Fig. 1 (a) ESI-Q-TOF MS/MS analysis of the SAX fraction No. 1 (*cf*. Fig. 1b in the article). Full-scan mass spectrum taken the TIC apex. The insets show the isotopic pattern of selenium at *m/z*= 285.04 ($[M+H]^+$) and the collision-induced dissociation (CID) spectrum of the pseudo-molecular ion. **(b)** Proposed fragmentation pathways of the Se-compound, selenohomolanthionine. For accurate mass information see Table 1 in the article.

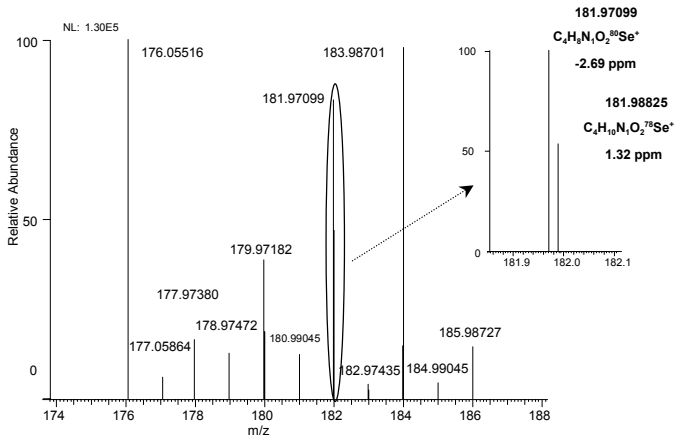
ESI Fig. 2



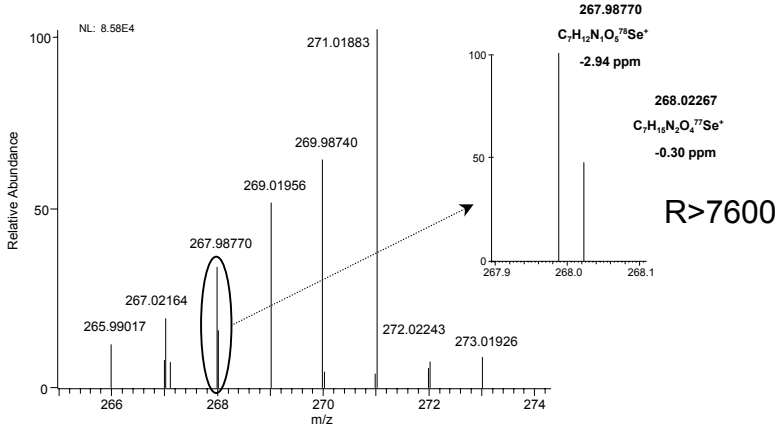
ESI Fig. 2 (a) ESI-Q-TOF MS/MS analysis of the SAX fraction No. 2 (*cf*. Fig. 1b in the article). Full-scan mass spectrum taken the TIC apex. The insets show the isotopic pattern of selenium at *m/z*= 400.04 ($[M+H]^+$) and the CID spectrum of the pseudo-molecular ion. **(b)** ESI-Q-TOF MS/MS analysis of the SAX fraction No. 3 (*cf*. Fig. 1b in the article). Full-scan mass spectrum taken the TIC apex. The insets show the isotopic pattern of selenium at *m/z*= 400.04 ($[M+H]^+$) and the CID spectrum of the pseudo-molecular ion. **(c)** Proposed fragmentation pathways of the detected Se-compound of SAX fraction No. 2, the isomer of γ-Glu-selenocystathionine. **(d)** Proposed fragmentation pathways of the detected Se-compound of SAX fraction No. 3, the isomer of γ-Glu-selenocystathionine. For accurate mass information see Table 1 in the article.

ESI Fig. 3

(a)

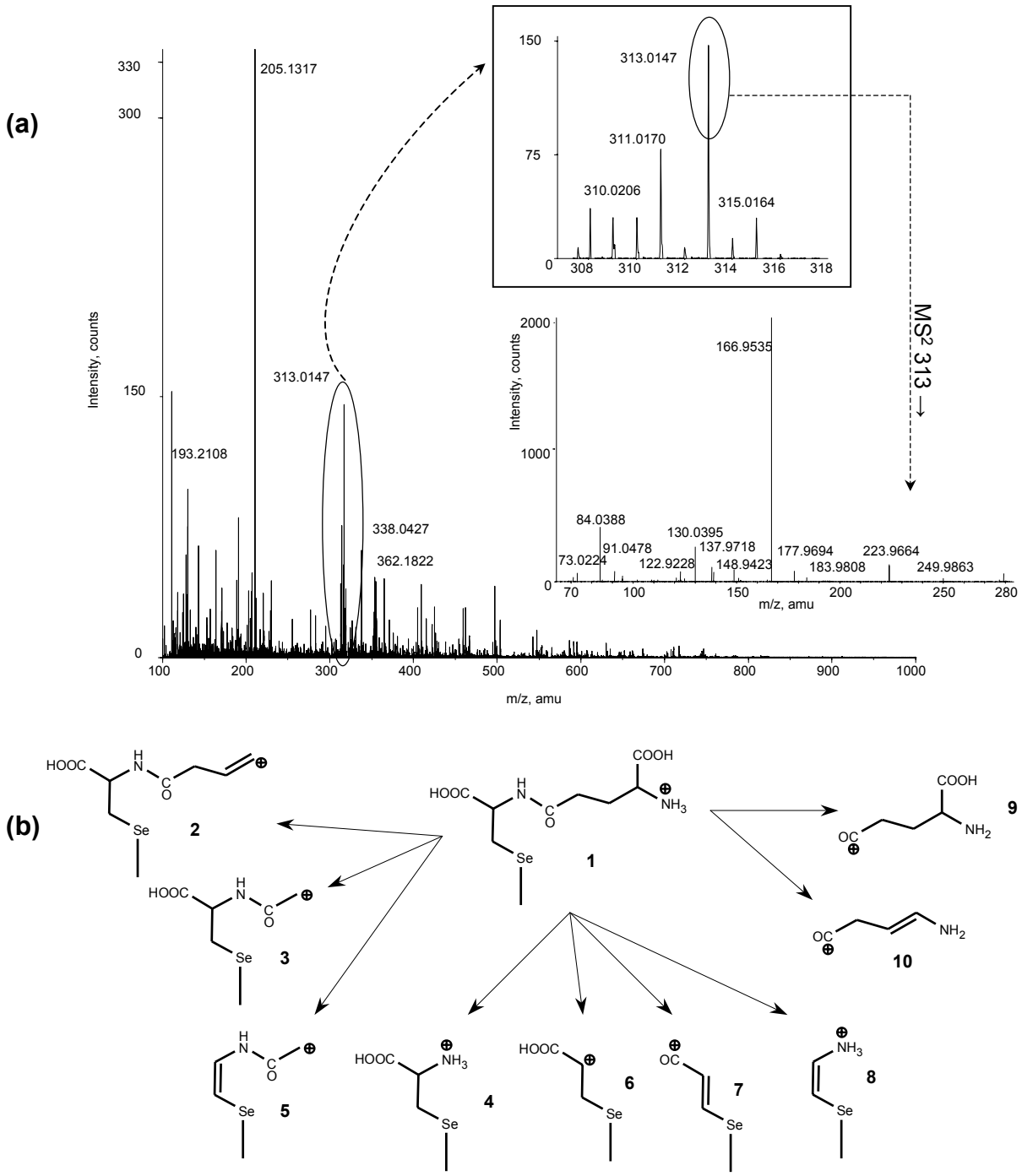


(b)



ESI Fig. 3 (a) and (b) Extracts of the HILIC-Orbitrap MS^n (n=2) spectra of the Se-species detected in the SAX fraction No. 4., *m/z* = 359.03519 (for details, see Fig. 3d in the article). The insets highlight the instrumental resolution required to detect and unambiguously identify the isotopes of different fragments.

ESI Fig. 4



ESI Fig. 4 (a) ESI-Q-TOF MS/MS analysis of the SAX fraction No. 6 (*cf*. Fig. 1b in the article). Full-scan mass spectrum taken the TIC apex. The insets show the isotopic patterns of selenium at *m/z*= 313.01 ($[M+H]^+$) and the CID spectrum of the pseudo-molecular ion. **(b)** Proposed fragmentation pathways of the Se-compound at *m/z*= 313.01, γ-Glu-*Se*-methylselenocysteine. For accurate mass information see Table 1 in the article.